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Weapons Systems Division
Systems Sciences Laboratory

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ABSTRACT

Nanometric aluminium grades such as *Alex* are known to react more rapidly than conventional aluminium grades in propellant and explosive compositions. To characterise *Alex,* and evaluate its influence upon near-field performance of explosive formulations, a series of velocity of detonation measurements and plate dent depth tests (detonation pressure) were performed on TNT/RDX/Al, TNT/Inert and Tritonal variants containing CAP45a and *Alex*. To clarify if the use of *Alex* reduced the critical diameters, critical diameter tests were performed on Tritonal variants. Modelling results with CHEETAH on heats of detonation, diameter effect and critical diameter are presented. Effects of adding different ingredients (inert ingredients, aluminium and high explosive such as RDX) are also discussed.

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Near-field Performance Evaluations of Alex Effect in Metallised Explosives

Executive Summary

Aluminium, which contributes to late energy releases in the detonation process, is commonly added to explosives to enhance both blast effects and underwater performance. Such aluminium grades, typically 10-20 micron in diameter, react predominantly during the expansion of the detonation products behind the reaction front, and behave largely as an inert material in the detonation front with little contribution of energy. However, Russian scientists [Reshetov et al 1984] who worked with *Alex* for a number of years, claimed that *Alex* contained significant additional "strain energy" above that chemically available which enabled it to greatly enhance the performance of both explosive and propellant systems. WSD initiated research into *Alex* in 1997 to investigate these claims. A bilateral program with Canada at the Defence Research Establishment Valcartier (DREV) to further examine the potential of *Alex* was established to evaluate its influence upon both near and far-field performance of explosive formulations. This report will give a summary of new and previously reported measurements of near-field performance evaluations, i.e., detonation velocity and plate dent depth tests and critical diameter tests.

To better understand the influence of *Alex* upon non-ideal detonation of TNT/Al explosives, the LLNL CHEETAH 2.0 code has been used to develop two models of aluminium combustion in the detonation front. The first approach employs traditional C-J detonation theory, and models particle size effects by limiting the amount of aluminium reacting in the detonation front. The second approach uses Wood-Kirkwood detonation theory with a Murnaghan equation of state for solid and liquid Al and Al_2O_3 to obtain kinetic rate laws for TNT and Al combustion. Modelling results with CHEETAH on heats of detonation, diameter effect and critical diameter are presented.

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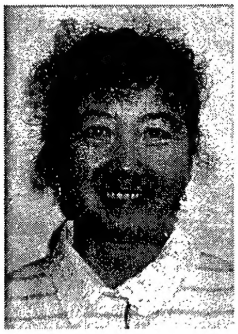
Authors



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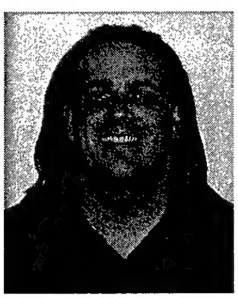
Weapons Systems Division

Jing Ping Lu was awarded a PhD in Civil Engineering at University of Wollongong in 1991. Before joining the Explosive Group, WSD at DSTO in March 2000, she was a senior research scientist in the Division of Building, Construction and Engineering, CSIRO where she spent 10 years working on modelling aspects of projects related to the structural use of different materials. She is currently conducting research into the performance prediction of explosive materials and the mathematical modelling and computer simulation of explosive behaviour.

Helen E. Dorsett
Weapons Systems Division

Helen Dorsett holds a BA in Physics from Rutgers University (USA), an MS in Chemical Physics and a PhD in Physical Chemistry from the University of Maryland (USA). She joined the Explosives Group in the Weapons Systems Division of DSTO in 1998 as a research scientist, where she performed computational studies of energetic molecules and small-scale testing of underwater explosives. She transferred to the Maritime Operations Division in 2001, where she currently undertakes mine warfare modelling in support of operational decision-making and tactical analysis.



Mark D. Franson
Weapons Systems Division

Mark joined Weapons Systems Division with a Bachelor of Applied Chemistry degree in 2002. He spent several years previously at the Ian Wark Research Institute (UniSA) conducting academic research into polymer science and surface modification. Currently Mark is working with the development of new polymer bonded explosives and NTO-containing explosive compositions, while studying toward his Masters degree in Defence Technologies.

Matthew D. Cliff
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Matthew Cliff completed his Honours degree at Deakin University in 1991 and his PhD in organic chemistry at the University of Wollongong in 1995. He commenced work at AMRL in 1996 and has worked on a range of tasks looking at new nitration methods, synthesis of energetic materials and PBX formulation and evaluation. In 1998/1999 he was attached to the Defence Evaluation and Research Agency, Fort Halstead in the UK and is currently conducting research into melt-castable Insensitive Munition fills and reactive metals for use in explosive formulations.

Contents

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1. Introduction

Aluminium, which contributes to late energy releases in the detonation process, is commonly added to explosives to enhance both blast effects and underwater performance. Such aluminium grades, typically 10-20 micron in diameter, react predominantly during the expansion of the detonation products behind the reaction front, and behave largely as an inert material in the detonation front with little contribution of energy. However, Russian scientists [Reshetov et al 1984] who worked with *Alex* for a number of years, claimed that *Alex* contained significant additional "strain energy" above that chemically available which enabled it to greatly enhance the performance of both explosive and propellant systems. WSD initiated research into *Alex* in 1997 to investigate these claims. A bilateral program with Canada (DREV) to further examine the potential of *Alex* was established to evaluate its influence upon near and far-field performance of explosive formulations. This report will give a summary of new and previously reported measurements of near-field performance evaluations, i.e., detonation velocity and plate dent depth tests and critical diameter tests. Different methods used for estimating detonation pressures are presented. Empirical relationships between pressures and parameters measured from plate-dent tests (dent depths, surface areas and volumes) are derived. Given that there is little work reported that allows the estimation of detonation pressures for *Alex*-based explosive formulations, the empirical equations described in this report will provide first approximation calculations of detonation pressures based solely on the dent depth data.

To better understand the influence of *Alex* upon non-ideal detonation of TNT/Al explosives, the LLNL CHEETAH 2.0 code has been used to develop two models of aluminium combustion in the detonation front. The first approach employs traditional C-J detonation theory, and models particle size effects by limiting the amount of aluminium reacting in the detonation front. The second approach uses Wood-Kirkwood detonation theory with a Murnaghan equation of state for solid and liquid Al and Al_2O_3 to obtain kinetic rate laws for TNT and Al combustion. Modelling results with CHEETAH on heats of detonation, diameter effect and critical diameter are presented.

2. Energetic Materials

2.1 Aluminium

The ultrafine aluminium used in these studies was *Alex* obtained from Argonide (USA). It was found that the batch of *Alex* contained approximately 9% aluminium nitride by X-ray diffraction analysis. *Alex* particle sizes ranged between 100 and 200nm. The reference conventional aluminium was Cap45a, sourced from Comalco Aluminium Powers, and having an average particle size of 17 μm [Cliff et al 2000].

Scanning electron micrographs of Cap45a and *Alex* are shown in Figure 1 [Cliff et al 2002].

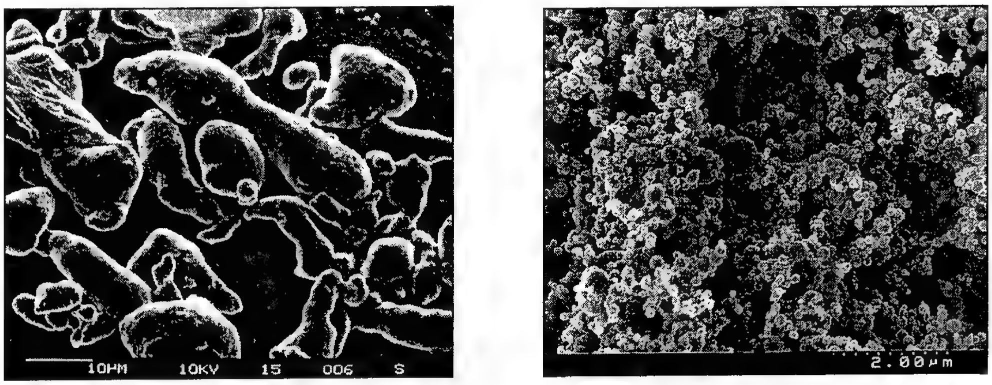


Figure 1. SEM photographs of aluminium powders. On the left is CAP45a (Australia); on the right, Alex (Argonide, USA). Note difference in scale.

2.2 Energetics

RDX Type I (Woolwich), Grade A [Australian Defence Standard 1996] and TNT flake [Australian Defence Standard 1987] were received from ADI Limited, Mulwala. RDX was received wet and oven dried at 60°C.

2.3 Explosive Formulations

TNT-based formulations were TNT/Graphite (80:20), TNT/LiF (80:20), Tritonal (80:20 TNT/Al) and TNT/RDX/Al (50:30:20) variants. For all formulations containing aluminium, the amount of aluminium was kept at 20% by weight. To ensure charge quality, a special casting technique was used with a heated rod (by hot fluid pumped through the rod) situated in the centre of the casting mould. The rod had to be lifted very slowly out of the casting over a period of time to eliminate the cracks and coring.

3. Experimental

3.1 VoD and Plate Dent Test

To characterise *Alex* and evaluate its influence upon near-field performance of explosive formulations, a series of velocity of detonation measurements and plate dent depth tests (detonation pressure) have been performed on TNT/Inert, TNT/RDX/Al and Tritonal variants containing Cap45a and *Alex*. All the compositions were cast into cylinders of length 250 mm, with diameters ranging from 50.5 to 81.91 mm. All the charges were fired unconfined, with detonation velocity measured by either digital streak photography (for most of the charges) or time-of-arrival piezoelectric pins spaced at 20.0 mm intervals along the length of the charge (for only 5 charges). Charges with diameters of 50.5 mm were fired in triplicate on a stack of three 150x150x50 mm

mild steel witness plates to record dent depths. The larger diameter charges were fired in duplicate on a stack of at least three 250x250x50 mm witness plates. Both small plates and large plates were each sourced from a single batch of 1018 cold rolled mild steel, Rockwell hardness B74-76 [Smith 1967]. The top plate was removed after each firing for dent volume, dent area and dent depth measurements. The middle and base backing plates were discarded as necessary to ensure a flat, undamaged surface obtained for each test. To provide reference detonation pressure, 6 Comp B charges and 3 TNT charges with diameters of 50.5 mm and 2 Comp B charges and 2 TNT charges with diameters of 74.82mm were also fired. The set-up is shown in Figure 2.

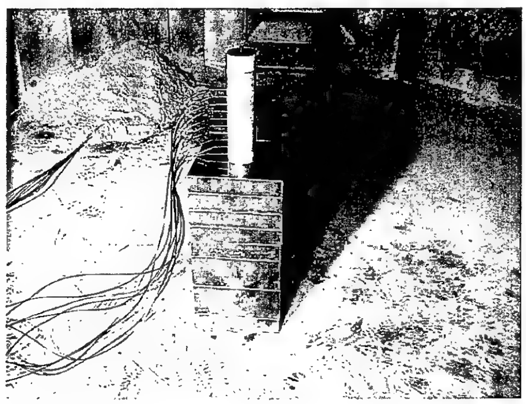


Figure 2. VoD /dent test set-up.

Figure 3 shows a typical example of the dented witness plates after testing. The witness plate data was measured on the new Sheffield - Endeavour Co-ordinate Measuring Machine (CMM). A series of points were taken over the affected areas of the plates. These points were saved as a DAT file that was imported into the CAD software UNIGRAPHICS. The points were then joined to create a surface that was fitted to the top of the plate forming a solid. The solid was then analysed for the volume and surface area. Table 1 shows the recorded experimental data including the data for the standard charges of TNT and Composition B. Figure 4 shows examples of the image frame and streak record of TNT/RDX/Al and TNT/Al detonation.

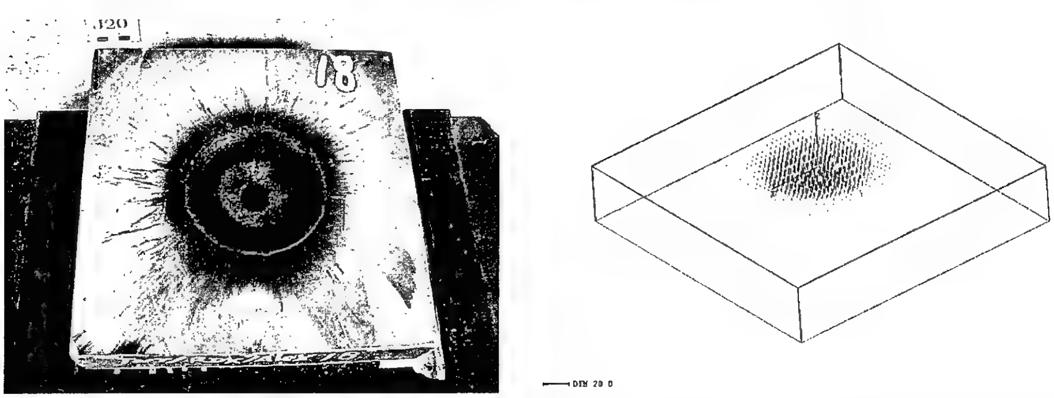
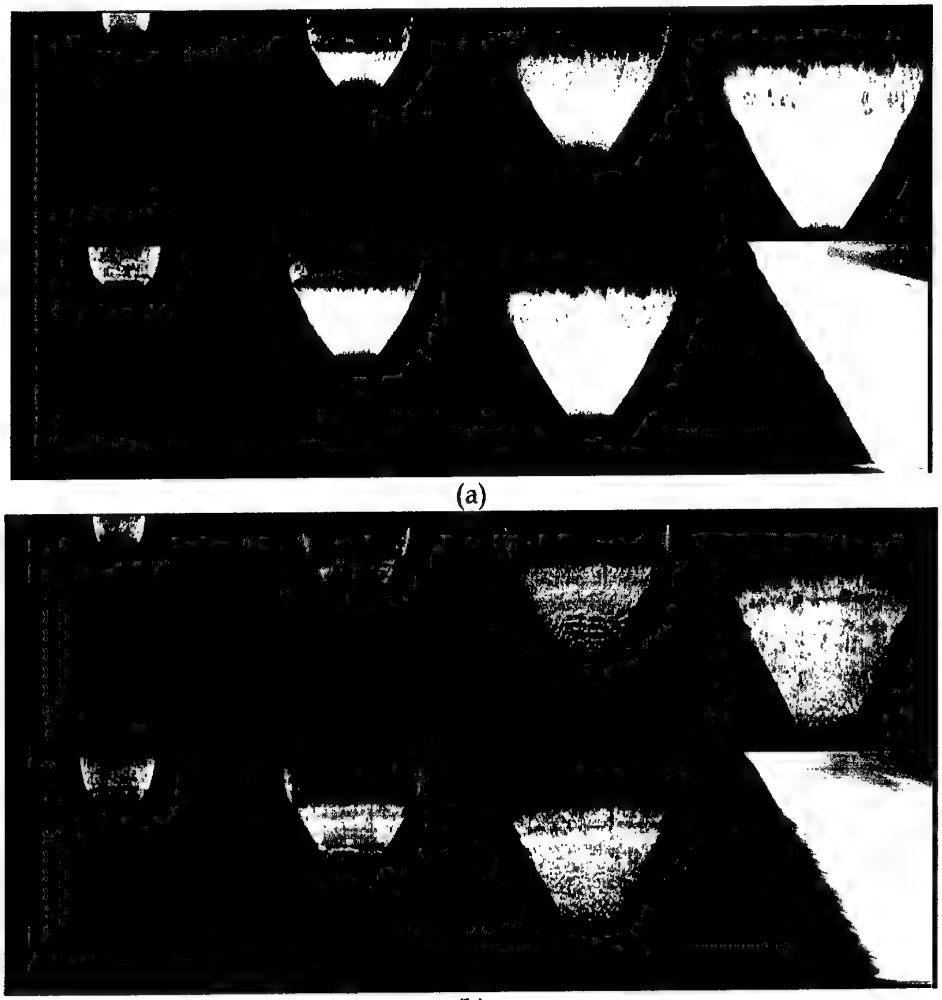


Figure 3. Dented witness plate after the test. On the left is the real plate; on the right is the sketch showing points for dent area and volume measurements.



(a)

(b)

Figure 4. Typical examples of the image frame and streak records of explosive detonation: (a) TNT/RDX/Al; (b) TNT/Al.

Table 1. Measured dent areas, dent volumes and dent depths.

Explosive	Diameter (mm)	Area (mm^2)	Volume (mm^3)	Depth (mm)
TNT/Alex	81.81	8421.15	56940.28	16.27
TNT/Alex	81.81	8183.22	55354.70	15.60
TNT/Alex	74.73	6884.92	40424.79	13.39
TNT/Alex	74.75	6607.36	39538.78	13.96
TNT/Al	81.90	7991.11	50710.37	13.65
TNT/Al	81.91	7695.56	47843.68	13.13
TNT/Al	74.83	6441.04	35263.75	11.53
TNT/Al	74.82	6314.82	35450.71	11.62
TNT/RDX/Alex	74.74	7806.00	54563.03	16.52
TNT/RDX/Alex	74.75	7529.30	53340.44	16.42
TNT/RDX/Al	74.79	7366.10	51045.63	15.02
TNT/RDX/Al	74.78	7478.92	51058.27	15.00
TNT/Graphite	50.50	2645.15	8666.35	7.19
TNT/Graphite	50.49	2605.55	8560.08	7.18
TNT/Graphite	50.45	2559.92	8481.19	7.09
TNT/LiF	50.45	2654.32	8910.81	7.17
TNT/LiF	50.45	2597.95	8815.99	7.21
TNT/LiF	50.45	2634.53	8959.98	7.13
Comp B	74.8	7758.54	55269.76	16.24
Comp B	74.76	7673.52	54523.46	15.75
Comp B	74.82	7686.99	55293.70	16.08
Comp B	50.24	3361.78	15498.13	10.38
Comp B	50.35	3430.83	15883.45	10.23
Comp B	50.37	3357.09	15634.62	10.10
Comp B	50.39	3360.82	15496.48	9.99
Comp B	50.40	3357.65	15485.64	10.11
Comp B	50.42	3352.31	15376.26	9.95
TNT	74.98	6439.29	36844.76	13.37
TNT	74.79	6801.88	38652.68	13.43
TNT	74.8	6518.61	37364.75	12.95
TNT	50.42	2832.78	10238.27	8.46
TNT	50.62	2825.25	10239.24	8.70
TNT	50.42	2826.32	10239.98	8.39

Averaged measured detonation velocity and dent depths for current data and previously reported data [Cliff et al 2002] are listed in Table 2.

Table 2. VoD and dent depth results for aluminised formulations.

Explosive	Charge dia (mm)	Al type	Density (g/cm^3)	VoD (m/s)	Dent depth (mm)
Tritonal	31.5	Cap45a	1.76	--	4.59
		Alex	1.78	–	5.00
	41.1	Cap45a	1.71	6427	5.95
		Alex	1.76	6722	7.20
	50.4	Cap45a	1.70	--	7.74
		Alex	1.69	–	9.93
	60.1	Cap45a	1.70	--	9.89
		Alex	1.69	--	11.96
	74.82	Cap45a	1.77	6855	11.58
		Alex	1.77	6998	13.68
	81.8	Cap45a	1.78	6905	13.39
		Alex	1.78	7019	15.94
TNT/RDX/Al	25.5	Cap45a	1.81	7047	4.34
		Alex	1.82	6806	4.62
	31.6	Cap45a	1.80	7042	5.47
		Alex	1.80	6754	6.08
	41.1	Cap45a	1.80	7111	7.25
		Alex	1.82	6855	8.12
	50.5	Cap45a	1.77	7039	9.50
		Alex	1.76	6665	10.04
	74.8	Cap45a	1.82	7433	15.01
		Alex	1.83	7029	16.47

3.2 Critical Diameter Tests

To clarify if the use of *Alex* reduced the critical diameters, critical diameter tests were performed on Tritonal variants. All the Tritonal variants were cast as at least 250mm long cylinders of various diameters. The diameters were of the 10-20mm range, stepped at approximately 2mm, and produced in triplicate. 50/50 Pentolite boosters for each of the charges were produced as right cylinders of corresponding diameters.

Preparation for firing involved attaching a booster and detonator holder to the end of a charge with glue, and holding the charge upright by taping it to a block of 200mm long pine. The charge was placed at the centre of a 100mm square x 10mm thick mild steel witness plate in the firing chamber. A RP-501 Economy EBW detonator (P/N 188-7359) was placed in the holder and wired for firing.

The firing of the charges was recorded with an Imacon 468 CCD digital camera. The VoD can be determined from the streak record facility of the camera.

For each Tritonal variant, the largest diameter was fired first. If a charge had a diameter greater than its critical diameter, the detonation front was carried through the whole 250mm length, and passed into the witness plate, leaving an obvious dent in the steel. Such a success of the charge to sustain a detonation was also confirmed by the camera data, and the result was labelled as a 'GO'. Each diameter was fired in triplicate, before moving on to the next smaller diameter. As the critical diameter was reached, the charge ceased to be able to carry the detonation front through the whole 250mm, and no dent was seen in the witness plate. The camera also showed the detonation front stopping part way along the length of the charge, leaving residual material. This failure of the charge to sustain a detonation was labelled as a 'NO GO'. Table 3 summarises the results of the critical diameter tests.

Table 3. Results of the Tritonal critical diameter tests on 250mm long cylinders.

Al type	Diameter of the cylinder					
	20mm	17.9mm	16.9mm	15.8mm	13.4mm	9.5mm
Cap45a	NO GO/NO GO/NO GO	NO GO	-	-	-	-
Alex	-	GO	GO/GO/GO	GO/GO/GO	GO/GO/GO	NO GO/NO GO/NO GO

4. Modelling with CHEETAH

4.1 Method

Calculations were performed with the CHEETAH 2.0 thermochemical code [Fried et al 1998]. C-J detonation calculations employed the BKW equations of state with BKWC and NEWC1 product libraries. 'Kinetic' calculations are based upon Wood-Kirkwood detonation theory, with a pressure-dependent rate law calibrated from experimental data.

4.2 Estimates from C-J Detonation Theory

Adopting the approach of Cowperthwaite [1993] and Anderson and Katsabanis [2000], we have calculated the heat of detonation for TNT/Al explosives by assuming some of the aluminium remains inert or "frozen" within in the detonation front. Calculations were first performed for TNT/Al 70/30 to compare with experimental results reported by Anderson and Katsabanis, and the results are presented in Table 4. A comparison of computed and experimental results suggests that approximately 66% of the Al is reacting with the detonation products in 70:30 TNT/Al formulations containing

"conventional" Al powder.[1] Better agreement is achieved when assuming an isentropic expansion to a moderate specific volume (1.9cc/g), and using the "NEWC1" library.

Table 4. Calculated and Experimental Heats of Detonation (cal/g) for 70:30 TNT/Al (ρ_0 = 1.88 g/cc, average Al particle diameter = 15 μm).

Composition	Amount of Al reacting	Products frozen at CJ		Products frozen at 1.9 cc/g		Expt.
		NEWC1	BKWC	NEWC1	BKWC	
70:30 TNT/Al	100%	1765	2062	1709	2042	1641 (1613)
	66%	1664	1814	1640	1668	
	50%	1453	1593	1369	1403	

We then calculated heats of detonation for 80:20 TNT/Al formulations containing either CAP45a or Alex. These results are presented in Table 5, together with the preliminary experimental results [Anderson 2001]. The calculated results for "conventional" 80:20 TNT/Al supports the finding of Anderson and Katsabanis that approximately 66% of the Al is reacting with the detonation products. In this case, better correlation with the experimental results is achieved when the products are frozen at the explosion state, rather than allowing an isentropic expansion to a moderate specific volume (1.9cc/g) as for TNT 70/Al 30.

Table 5. Calculated and Experimental Heats of Detonation (cal/g) for 80:20 TNT/Al.

Composition	Amount of Al reacting	NEWC1					
		Products frozen at CJ			Products frozen at 1.9cc/g		
		Cal.	Exp.	Err. %	Cal.	Exp.	Err. %
80:20 TNT/Cap45a (ρ_0= 1.71 g/cc)	100%	1668	1412	18.1	1718	1412	21.7
	66%	1445		2.3	1361		-3.6
	50%	1318		-6.7	1204		-14.7
80:20 TNT/Alex (ρ_0= 1.76 g/cc)	100%	1693	1438	17.7	1719	1438	19.5
	66%	1456		1.3	1369		-4.8
	50%	1330		-7.5	1210		-15.9

Interestingly, using the "frozen" Al approximation, CHEETAH calculations predict that like TNT/Cap45a, only about 66% of Alex will react in the detonation zone as well. However, some care is required to interpret this result, since Alex powders contain only 85% active aluminium as compared with Cap45a, which is 99% active aluminium

[1] The aluminium powder used in these formulations is Valimet H-15, with an average particle diameter of 15 μm.

[Berry et al 2002]. Hence, at least 76% of Alex is required to react to yield the equivalent of 66% reaction in Cap45a.

4.3 Rate Laws from Kinetic Detonation Theory

Kinetic CHEETAH is based on the Wood-Kirkwood (WK) detonation theory [Wood and Kirkwood 1954] which is specially designed for modelling time-dependent phenomenon. The new chemical kinetics model implemented in CHEETAH considers detonation in composite explosives with large reaction zones, and the interplay between the energy produced by kinetically controlled reactions and the energy lost due to radial expansion of the product gases. Wood-Kirkwood theory thus allows prediction of the dependence of detonation parameters on charge diameters, and estimation of the length of the detonation zone, identified as the region behind the detonation wave for which the sum of the mass velocity and the velocity of sound is equal to the detonation velocity [Loboiko and Lubyatinsky 2000].

As described in the CHEETAH 2.0 User's Manual [Fried et al 1998], WK theory starts with the hydrodynamic Euler equations coupled to chemical kinetics. The theory treats the detonation along the centre of the cylinder. Radial expansion is treated as a first order perturbation to perfect one dimensional planar detonation. The Euler equations are reduced to their steady state form. The result is a set of ordinary differential equations that describe hydrodynamic variables and chemical concentrations along the centre of the cylinder. The theory requires specification of the rate of radial expansion, ω_r, as a function of radius. Although Kinetic CHEETAH has implemented three radial expansion models in the code, in this study the simple pressure model with the following time rate of change of ω_r is used:

$$\frac{d\,\omega_r}{dt} = \frac{2SP}{R_o^2 \rho_o} - S\,\omega_r^2 \tag{1}$$

where
$$\omega_r(t=0) = (D_s - u)/R_c \tag{2}$$

Here, P is the pressure, u is the particle velocity in the shock frame, ρ_o is the initial density of the explosive, R_o is the charge radius and S is an empirical scaling factor. If this model is used with $S = 0$, ω_r is a constant with the initial value determined by the radius of curvature R_c, the detonation velocity D_s, and the particle velocity at the detonation front. The radius of curvature is obtained from Souer's detonation front curvature and size effect data [Souers 1998].

Kinetic CHEETAH assumes the concentrations of individual reactants are controlled by the rate of the kinetic reactions, while the products are assumed to be in thermochemical equilibrium. Kinetic CHEETAH supports multiple reaction rate laws:

- Simple constant reaction rate law
- Simple Arrhenius kinetics with a temperature-dependent pre-factor

- Pressure-dependent rate law
- Hot spot model

CHEETAH has used the following simple pressure-dependent rate law to infer kinetic rates for a variety of high explosives and their composites:

$$d\lambda/_{dt} = (1-\lambda)\,R\,P^{D} \qquad (3)$$

where R is the rate constant, D is the pressure exponent and λ represents the amount of unburned reactant normalised to vary between zero (all unburned) and one (all burned).

We have also used the same rate law in our study to model the aluminium combustion, which is appropriate to a surface-controlled reaction. Rate constants for the reaction of individual TNT and Al components have been developed by calibrating kinetic parameters to experimental data [Brousseau and Cliff 2001], and are listed in Table 6. Note that these constants are different from both those listed in the CHEETAH 2.0 User's Manual and the updated values defined by Howard et al. [1999].

Table 6. Rate constant R used in pressure-dependent rate laws.

Reactant	R ($\mu s^{-1}GPa^{-2}$)		
	CHEETAH 2.0	Howard et al.	This study
Al	0.0075	0.0075	0.002
TNT	0.03	0.1	0.15

Figure 5 summarises kinetic CHEETAH predictions of detonation velocities as a function of Al concentration and particle size using the NEWC1 product library, compared with the experimental data of Shepherd [1956] and Brousseau and Cliff [2001]. It can be seen that CHEETAH predictions simulate the general trend of decreasing detonation velocity with increasing the amount of Al in the formulation for the largest particle size (125 μm). As discussed by Howard et al [1999], a simple surface area scaling of the rate would predict that only a relatively small fraction of the Al reacts in the detonation wave, and does not replicate the Al particle-size dependence of the detonation velocity. This contrasts with the observed increase in detonation velocity with higher *Alex* concentrations which suggest that *Alex* reacts in the detonation front.

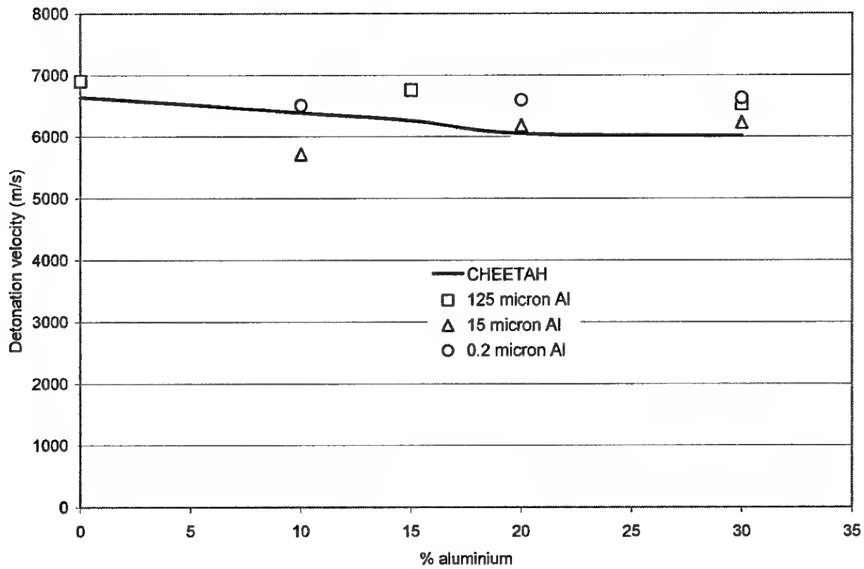


Figure 5. Detonation velocities for TNT/Al formulations as a function of Al concentration.

4.4 Effect of Diameter on Detonation Velocity

Figure 6 summarises kinetic CHEETAH predictions (with the NEWC1 product library) of detonation velocity as a function of reciprocal of diameter, plotted with the experimental data of Brousseau and Cliff [2001]. CHEETAH is found to qualitatively reproduce the trend of diameter dependence, however, to date, no set of reaction parameters has been found to reproduce exactly the observed diameter/detonation velocity dependence.

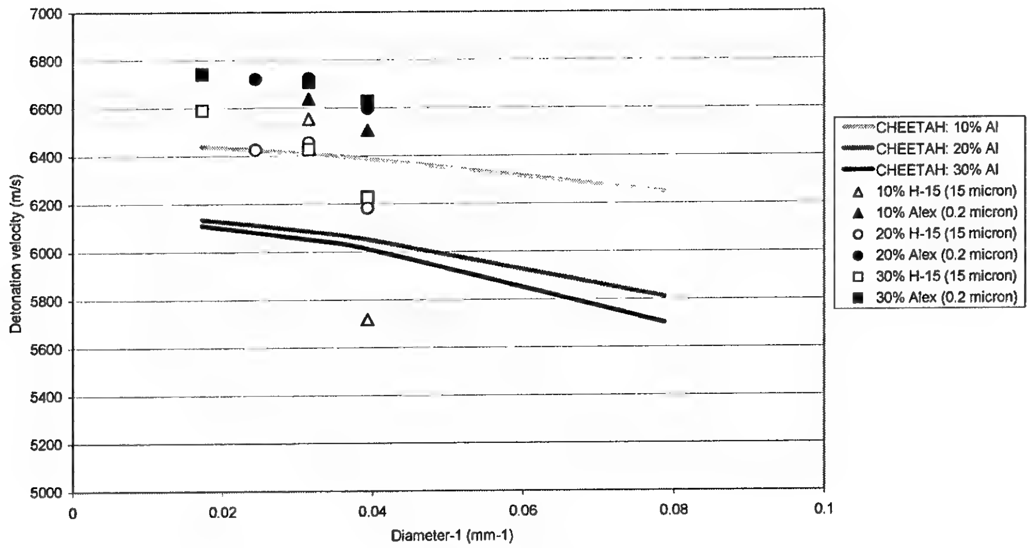


Figure 6. Detonation velocity versus reciprocal diameter of TNT/Al formulations.

4.5 Critical Diameter

According to Cooper [1996], side losses that cause steady-state detonation velocity to decrease in the non-ideal region, eventually become so dominant with decreasing diameter that a point is reached where steady-state detonation cannot be maintained. This point is called the failure diameter or the critical diameter. Critical diameter is strongly affected by confinement, particle size, initial density, and ambient temperature of the unreacted explosive. Decreasing particle or grain size also decreases critical diameter. Figure 7 presents the detonation velocity versus charge diameter curve for Tritonal predicted by Kinetic CHEETAH with the rate constants for the reaction of individual TNT and Al components developed in this study. The sharp decrease in detonation velocity at charge diameter less than 23mm is in agreement with the test results presented in this report for Tritonal with traditional aluminium Cap45a (20mm < critical diameter < 25.4mm). This is also consistent with the reported critical diameters of 18.3mm [Hall and Holden, 1988] and 20mm [Brousseau et al, 2002] for Tritonal.

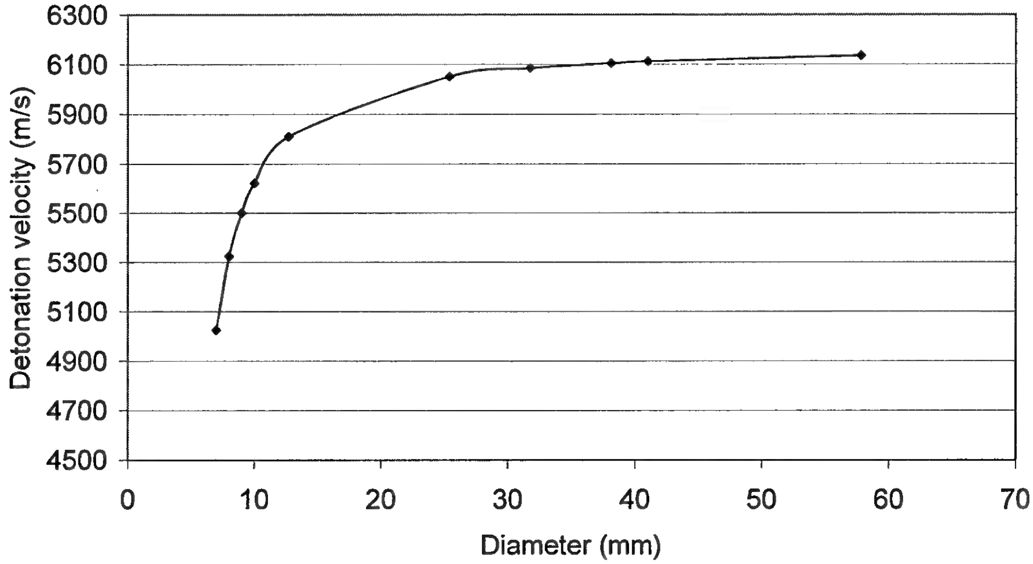


Figure 7. Detonation velocity versus charge diameter of Tritonal.

5. Alex Effect on Near-field Performance Formulas

5.1 Detonation Velocity

The observed increases in detonation velocities of TNT/Al and TNT/RDX/Al charges containing Alex are shown in Figure 8. Due to charge qualities of 50mm diameter for TNT/RDX/Al formulation, the detonation velocity is unrealistically low, which is not included in the plots.

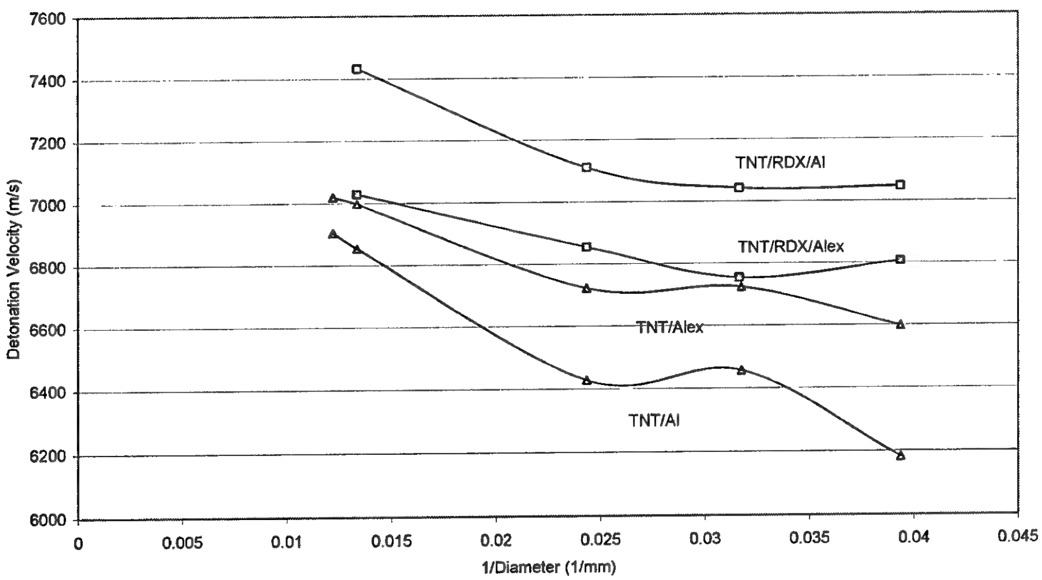


Figure 8. Increases in detonation velocities of TNT/Al and TNT/RDX/Al Charges containing Alex.

TNT/Al charges containing *Alex* show significantly higher detonation velocities than those containing Cap45a. Measured detonation velocities are consistently higher for *Alex*-based formulations over the range of weight percentage ratios tested. These results suggest that the *Alex* burns fast enough to contribute energy to the detonation front, thereby increasing detonation velocity.

TNT/RDX/Al formulations containing Alex have lower detonation velocities than those containing conventional aluminium. According to Brousseau and Cliff [2001], the reaction rate in TNT/RDX/Al formulations must be such that Alex reacts just fast enough to enhance the brisance (see the increase in detonation pressure described in the following section) and not the reaction front (velocity of detonation). A better analysis of the energy-release mechanisms in the near-field should provide an explanation to this phenomenon.

5.2 Detonation Pressure and Dent Depth

Given that there is little work reported that allows the estimation of detonation pressures for *Alex*-based explosive formulations, the empirical equations described in a separate technical note [Lu et al 2003] will provide first approximation calculations of detonation pressures based either solely on the dent depth data or on both dent depth data and detonation velocity data. The empirical formula based solely on the dent depth data for the available experimental data region $0.28<d_s<0.58$ is:

$$P_{cj} = -131.14 d_s^2 + 167.99 d_s - 22.243 \quad (4)$$

Where

P_{cj} = detonation pressure (GPa)

$d_s = d/r$ (scaled dent depth) (d is the dent depth and r the radius of the charge)

Figure 9 presents the detonation pressures estimated with equation (4) versus charge diameters for TNT/Al and TNT/RDX/Al explosive formulations. Both TNT/Al charges and TNT/RDX/Al charges containing *Alex* show significantly higher detonation pressures formulations. It also shows that the relative improvement in detonation pressures of TNT/Al and TNT/RDX/Al formulations depends upon the charge diameters. For TNT/Al formulations, experiments were performed on charges close to the critical diameter of Tritonal (D_{crit} = 18.3 mm [Hall and Holden 1988]), hence measurements were taken in a region of highly non-ideal detonation behaviour.

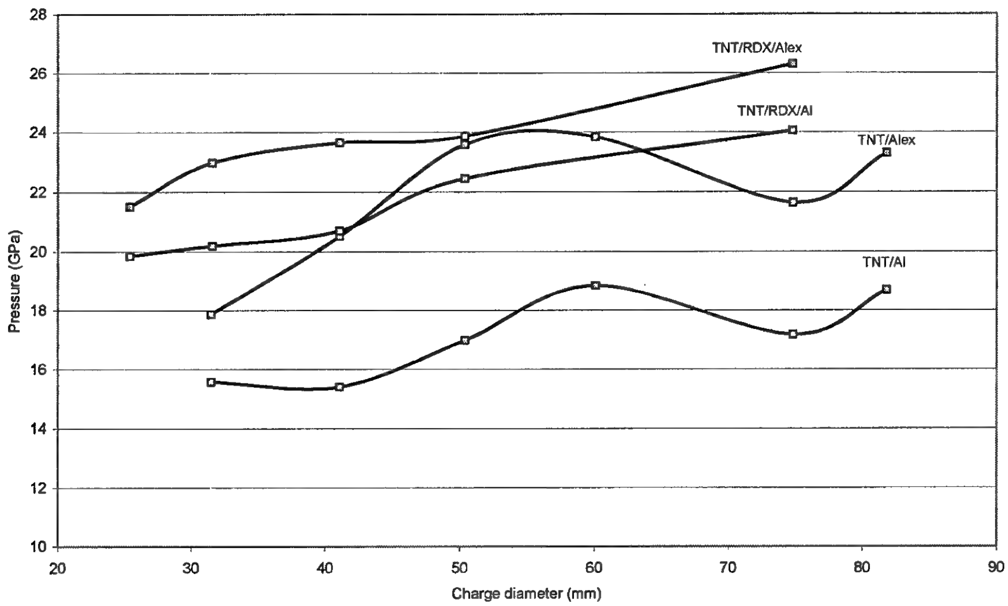


Figure 9. Detonation pressure versus charge diameter of TNT/Al and TNT/RDX/Al.

The increases in dent depths of TNT/Al and TNT/RDX/Al charges containing *Alex* are shown in Figure 10. Following the same trend as detonation pressure, both TNT/Al charges and TNT/RDX/Al charges containing *Alex* show significantly higher dent depths than those containing Cap45a, although the increases are generally larger for the TNT/Al formulations (Figure 10), which are diameter dependent.

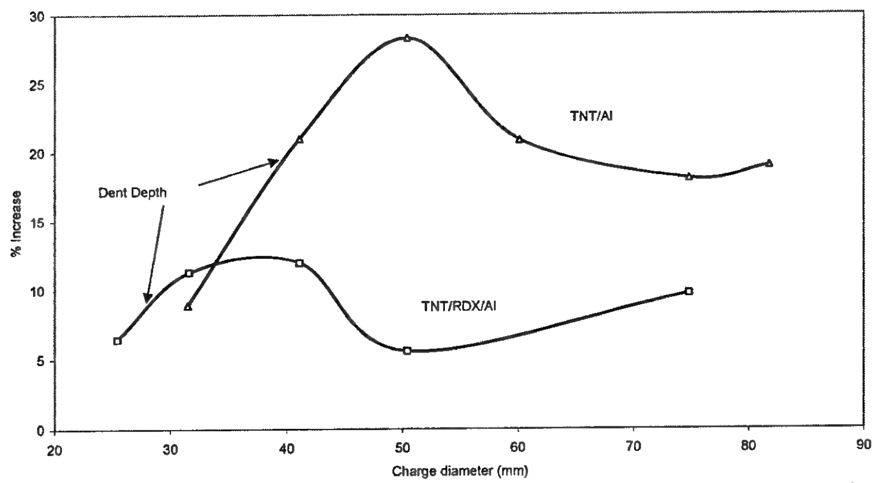


Figure 10. Increases in dent depths of TNT/Al and TNT/RDX/Al Charges containing Alex.

5.3 Critical Diameter

Referring to Table 3 and the previous results [Cliff et al 2000] showing that the TNT/Cap45a charges detonated at 25.4mm, it indicated that the critical diameter for TNT/Cap45a charges was between 20mm and 25.4mm. The critical diameter for TNT/Alex charges was between 9.5mm and 13.4mm. The current test results supports the conclusion of [Brousseau et al, 2002] that the critical diameter appears to be reduced significantly by the use of *Alex* for Tritonal.

6. Effects of Adding Different Ingredients on Pressures of TNT Formulations

Table 7 compares the pressures estimated from plate dent tests based on different calibrations (dent volumes, dent areas and dent depths) with those calculated by CHEETAH. Figures 11 and 12 plot the pressures estimated from plate dent tests based on dent depth calibrations with those calculated by CHEETAH for 75mm and 50mm charges respectively. In general, CHEETAH predictions show good agreement with experimental data. With the exception of TNT/Alex formulations, CHEETAH significantly underestimates the detonation pressures for charges at diameters of 81.81mm and 50.4mm, but it gives much better correlation with experimental data for charges at diameters of 74.74mm. As CHEETAH calculations are based on assumptions that the charge diameters are infinitely large without reflecting the charge diameter effect, it is understandable for the predicted pressures to be less than those observed in

experimental for the smaller charges at diameters of 50.4mm. However, the reason for the discrepancy for the larger charges at diameters of 81.81mm is not clear.

Table 7. Comparison of pressures estimated from plate dent tests with those calculated by CHEETAH.

Name	Diameter (mm)	Density (g/cc)	Plate Batch	Pressure (GPa)			
				CHEETAH	Exp.		
					P_v	P_A	P_d
TNT	74.86	1.56	Large	18.65	18.4	18.4	18.4
CompB	74.79	1.68		27.41	26.7	26.7	26.7
TNT/Alex	81.81	1.78		19.23	27.35	25.8	24.34
	74.74	1.78		19.23	19.47	20.96	20.88
TNT/Al	81.91	1.78		18.39	24	24.37	20.45
	74.82	1.77		18.39	17.22	19.82	17.68
TNT/RDX/Alex	74.74	1.82		24.2	26.28	23.83	25.15
TNT/RDX/Al	74.79	1.83		23.45	24.86	23.06	22.92
TNT	50.49	1.57	Small	18.67	18.4	18.4	18.4
CompB	50.36	1.685		27.67	26.7	26.7	26.7
TNT/Graph	50.48	1.71		15.77	15.4	16.94	15.39
TNT/LiF	50.44	1.73		16.77	15.4	16.94	15.49
TNT/Alex	50.4	1.69		17.79	-	-	23.82
TNT/Al	50.4	1.7		16.53	-	-	18.56
TNT/RDX/Alex	50.5	1.76		22.13	-	-	24.08
TNT/RDX/Al	50.5	1.77		21.15	-	-	22.79

Note: P_v for calibrations based on dent volumes, P_A for calibrations based on dent areas and P_d for calibrations based on dent depths.

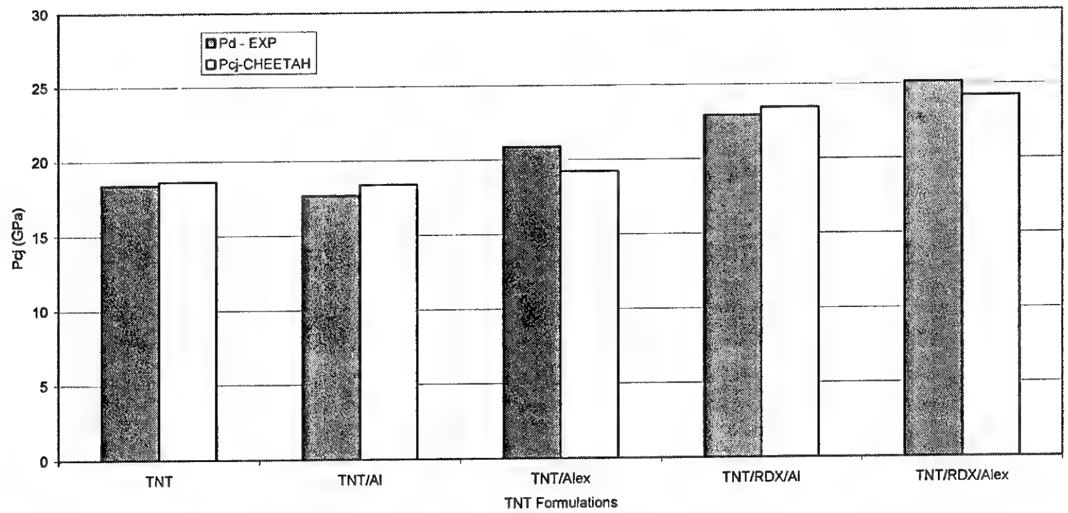


Figure 11. Pressure versus different ingredients added to the TNT formulations for 75mm charges.

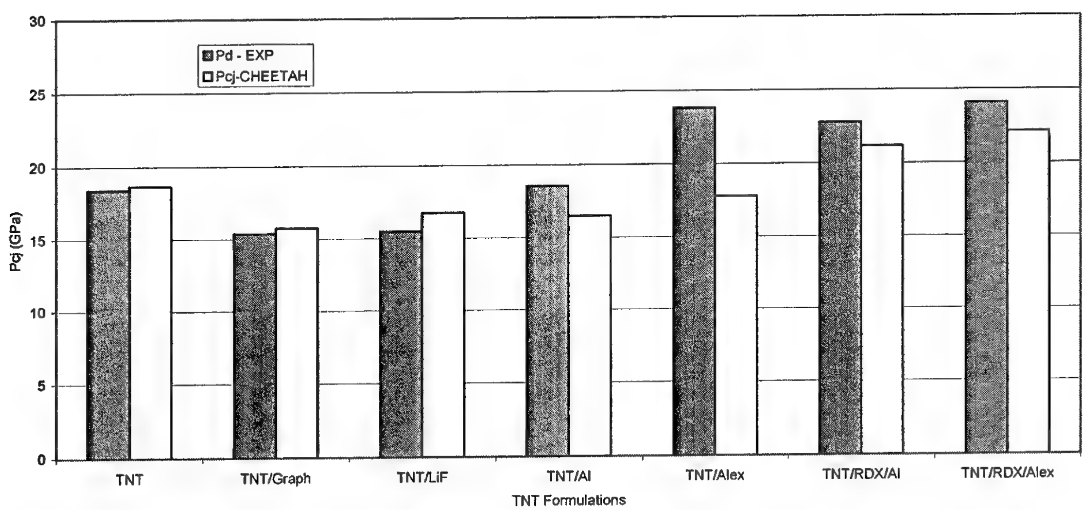


Figure 12. Pressure versus different ingredients added to the TNT formulations for 50mm charges.

The results in Table 7 and Figures 11 and 12 also show different effects of adding different ingredients in detonation pressures of TNT formulations. As expected, inert ingredients Graphite and Lithium Fluoride reduce TNT detonation pressures. The pressures for the TNT/inert composite are lower than the corresponding ones with the 80/20 TNT/Al composite. This supports the finding of Shepherd [1956] that aluminium, though largely inert in the wave front, does play a minor part in the reaction of the under-oxidised TNT. In both large and small diameters studied, the pressures for TNT/Alex and TNT/RDX/Alex (50/30/20) formulations are higher than the corresponding ones with the TNT/Al and TNT/RDX/Al formulations. This indicates that *Alex* reacts fast enough to contribute energy to the wave front and plays a significant part in the reaction of the under-oxidised TNT. TNT/RDX/Alex and TNT/RDX/Al formulations have the highest pressures for all TNT formulations at a nominal diameter of 75mm, whereas at a nominal diameter of 50mm they have the similar pressures as TNT/Alex formulations.

7. Conclusions and Future Directions

From the modelling and experimental studies outlined previously, the following conclusions have been reached.

- The results of the detonation velocity and plate dent tests show that TNT/Al charges containing *Alex* have significantly higher detonation velocities than those containing Cap45a. TNT/RDX/Al formulations containing *Alex* have lower detonation velocities than those containing conventional aluminium. Both TNT/Al charges and TNT/RDX/Al charges containing *Alex* show significantly higher detonation pressures than those containing Cap45a, although the increases are generally larger for the TNT/Al formulations. It also shows that the relative improvement in detonation pressures of TNT/Al and TNT/RDX/Al formulations depends upon the charge diameters.
- The consistent high detonation velocities for various *Alex* contents at different charge diameters in the experimental data support that the *Alex* appears to react in the detonation front in the TNT-based compositions.
- Critical diameter tests were carried out on Tritonal variants containing Cap45a and *Alex*. The critical diameter for TNT/Cap45a charges was between 20mm and 25.4mm. The critical diameter for TNT/Alex charges was between 9.5mm and 13.4mm. The critical diameter appears to be reduced significantly by the use of *Alex*.
- Inert ingredients Graphite and Lithium Fluoride reduce TNT detonation pressures.
- The finding of higher pressures for TNT/Alex and TNT/RDX/Alex (50/30/20) formulations than the corresponding ones with the TNT/Al and TNT/RDX/Al formulations indicates that Alex reacts fast enough to contribute energy to the wave front and plays a significant part in the reaction of the under-oxidised TNT.

- The comparison between computed and experimental heat of detonation for TNT 80/Al 20 confirms the finding of Anderson and Katsabanis that approximately 66% of the Al is reacting with the detonation products in TNT/Al composition. Better correlation with the experimental results is achieved when assuming the products frozen at the explosion state.
- The calculations with the "NEWC1" library in CHEETAH correlate most closely with the experimental data.
- Kinetic CHEETAH with a pressure-dependent rate law can predict the general trend of the detonation velocity versus diameter effect, but it can not replicate the Al particle-size dependent of the detonation velocity.
- The sharp decrease in detonation velocity at charge diameter less than 20mm predicted by Kinetic CHEETAH is in agreement with the test results presented in this report for Tritonal with traditional aluminium. This is also consistent with the literature reported critical diameters for Tritonal.

It is recommended that the following areas be considered for the future work.

- Use Hugoniot data to fit JWL equation of state parameters for un-reacted TNT/Al explosives.
- Use CHEETAH to determine pressure versus volume data for products and then fit the data to derive approximate JWL equation of state parameters for products.
- Use the above JWL equations of state as input data for LS-DYNA and develop an Ignition and Growth Reactive Model for TNT/Al formulations to study the role of aluminium and particle size effects.
- Apply the Ignition and Growth Reactive Model to simulating aquarium tests of *Alex*-based Tritonal using different growth rates for *Alex* and Al.

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19. ABSTRACT

Nanometric aluminium grades such as Alex are known to react more rapidly than conventional aluminium grades in propellant and explosive compositions. To characterise Alex, and evaluate its influence upon near-field performance of explosive formulations, a series of velocity of detonation measurements and plate dent depth tests (detonation pressure) were performed on TNT/RDX/Al, TNT/Inert and Tritonal variants containing CAP45a and Alex. To clarify if the use of Alex reduced the critical diameters, critical diameter tests were performed on Tritonal variants. Modelling results with CHEETAH on heats of detonation, diameter effect and critical diameter are presented. Effects of adding different ingredients (inert ingredients, aluminium and high explosive such as RDX) are also discussed.